

On the cutoff parameter in the translation-invariant theory of the strong coupling polaron. (response to comments [8] on the paper V. D. Lakhno, SSC, 152, (2012), 621)

V.D. Lakhno^{a,*}

^a*Institute of Mathematical Problems of Biology, Russian Academy of Sciences, Pushchino, Moscow Region, 142290, Russia*

Abstract

The paper is a reply to the arguments adduced by the authors of [8] against the results obtained by the author in [6, 7]. It is shown that these arguments are based on the erroneous approach made in [8] to the strong coupling limit when the cutoff parameter is introduced in the theory.

Keywords: cutoff parameter, bipolaron, Tulub approach

Historically, the polaron theory was among the first to be developed for the description of interaction between a particle and a field. Being nonrelativistic, it did not involve the cutoff parameter which is an inherent attribute of relativistic quantum theories for the particle-field interaction. For this reason the polaron theory has been a ground for testing various quantum field methods.

Among the fundamental problems which have been discussed throughout the whole history of the polaron theory development is that of whether the polaron is localized or delocalized in the strong coupling limit [1]-[5]. In my recent papers [6, 7] I have shown that the ground state of the polaron and bipolaron is delocalized since its energy value was found to be lower than that of the localized one. The approach used in [6, 7] which eliminates the particle's coordinates through canonical transformation and therefore is translation invariant by itself, leads to a delocalized state for all the coupling constants α , including the limit case $\alpha \rightarrow \infty$.

In recent comments on these papers [8] a conclusion was made about their fallacy. Here we reply to the arguments adduced in [8].

The results obtained in [6, 7] are based on the approach [9] developed by Tulub for describing the strong coupling polaron. Tulub's theory involves the function $q(1/\lambda)$ (Q in designations used in [8]) where $\lambda = 4\alpha a/3\sqrt{2\pi}$, α is the constant of electron-phonon coupling, a is a variational parameter. Tulub found $q(0) = 5,75$. At the same time the authors of [8] showed that q is a monotonously increasing function of λ and as $\lambda \rightarrow \infty$ $q(1/\lambda) \rightarrow \infty$. They considered the value $q(0) = 5,75$ to be "non-physical" and used the asymptotics $q(1/\lambda) = 2\sqrt{3\lambda}$ as the basis for their calculations of the polaron energy. As a result they obtained the energy $E \sim \alpha^{4/3}$ which depends on α weaker than the well-known strong coupling limit $E \sim \alpha^2$. Therefore the values of the polaron energy in [8] are greater than those

found in the strong coupling theory. So strange behavior of the function $q(1/\lambda)$ uncharacteristic for physical systems has not got the attention of the authors of [8].

Turning to the root of the matter, we note that Tulub's theory is a quantum field polaron theory in which the cutoff parameter arises naturally.

To demonstrate this fact let us choose the probe functions f_k involved in [9] in the form:

$$f_k = -\theta(k_{max} - k) V_k \exp(k^2/a^2), \quad (1)$$

where $\theta(x) = 1$, $x > 0$ and $\theta(x) = 0$, $x < 0$. For $k_{max} = \infty$, f_k are the functions chosen in [9]. With the use of (1) Tulub's function $q(1/\lambda)$ will be written as

$$q(1/\lambda) = \frac{2}{\sqrt{\pi}} \int_0^{y_{max}} \frac{e^{-y^2}(1 - \Omega(y))dy}{(1/\lambda + V(y))^2 + \pi y^2 e^{-2y^2}/4}, \quad (2)$$

$$\Omega(y) = 2y^2 \left\{ (1 + 2y^2)ye^{y^2} \int_y^\infty e^{-t^2} dt - y^2 \right\},$$

$$V(y) = 1 - ye^{-y^2} \int_0^y e^{t^2} dt - ye^{y^2} \int_y^\infty e^{-t^2} dt,$$

where $y = k/a$, $y_{max} = k_{max}/a$. In Tulub's paper the upper limit of integration in (2) was chosen to lie in the range

$$a \ll k_{max} \ll a\sqrt{\lambda} \quad (3)$$

This choice of the cutoff parameter is caused by the fact that for $y \rightarrow \infty$, $V(y) \rightarrow -3/4y^4$ and integration in (2) must not involve the maximum of the integrand function occurring at the point $y_0 = \sqrt[4]{3\lambda}/4$, since for $\alpha \rightarrow \infty$ $y_0 \rightarrow \infty$ (see marginalia at page 1833 in Tulub's paper [9]). When the cutoff parameter lies in the range (3), the value of q in [9] was found to be $q = q(0) = 5,75$. This leads to the polaron energy $E = -0,105\alpha^2$.

*Corresponding author

Email address: lak@impb.psn.ru (V.D. Lakhno)

The problem which remains to be clarified is whether condition (3) is consistent with the limit $\alpha \rightarrow \infty$. If we admit that it is, the quantity a will be: $a \sim \alpha$ [9].

Expressions for α and (3) yield that for $k_{max} \sim \alpha^p$ the value of k_{max} can always be chosen so that condition (3) be fulfilled for any p lying in the range $1 < p < p_1$, where $p_1 = 3/2$. This proves the correctness of inequalities (3).

For $p > p_1$ conditions (3) fail and integration in (2) involves the maximum of the integrand lying on the infinity (as $\alpha \rightarrow \infty$). The value of q becomes equal to $q(1/\lambda) = 2\sqrt{3\lambda}$ and the polaron energy is $E \sim \alpha^{4/3}$ as was found in [8].

Hence, in theory [9] the variational estimate of the ground state energy greatly depends on the choice of the probe function f_k . It can be said that Tulub's choice of f_k is the best (see however comment [10]). On the contrary, the choice of f_k made in [8] is the worst.

Notice that earlier the fact that the strong coupling limit depends on the form of the relation between the cutoff parameter and the constant of the electron-phonon interaction was pointed out in paper by Gross [3]. All the aforesaid suggests that depending on the value of p , q can take on any value in the range $q \in (5, 75 \div \infty)$, as $\alpha \rightarrow \infty$. In the case of $q = 5, 75$ the polaron value will be the lowest. Hence, presently the translation-invariant approach developed in [9] is the best. For the polaron (bipolaron), it yields lower variational estimates of the ground state energy, as $\alpha \rightarrow \infty$, than theories with spontaneously broken symmetry do (discussion of these problems is given in [11]), and the results obtained in [6, 7] raise no doubt.

The work was supported by the Russian Foundation for Basic Research, project N 11-07-12054 and 10-07-00112.

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